

1000562

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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Jan 25 BLAST(R) searching in REGISTRY available in STN on the Web
NEWS 3 Jan 29 FSTA has been reloaded and moves to weekly updates
NEWS 4 Feb 01 DKILIT now produced by FIZ Karlsruhe and has a new update frequency
NEWS 5 Feb 19 Access via Tymnet and SprintNet Eliminated Effective 3/31/02
NEWS 6 Mar 08 Gene Names now available in BIOSIS
NEWS 7 Mar 22 TOXLIT no longer available
NEWS 8 Mar 22 TRCTHERMO no longer available
NEWS 9 Mar 28 US Provisional Priorities searched with P in CA/CAPLUS and USPATFULL
NEWS 10 Mar 28 LIPINSKI/CALC added for property searching in REGISTRY
NEWS 11 Apr 02 PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead.
NEWS 12 Apr 08 "Ask CAS" for self-help around the clock
NEWS 13 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 14 Apr 09 ZDB will be removed from STN
NEWS 15 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 16 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 17 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 18 Apr 22 Federal Research in Progress (FEDRIP) now available

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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NEWS WWW CAS World Wide Web Site (general information)

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Kamal Saeed

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COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

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DICTIONARY FILE UPDATES: 7 MAY 2002 HIGHEST RN 412267-09-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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=>
Uploading C:\Program Files\Stnexp\Queries\0989932211.str

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> s l1
SAMPLE SEARCH INITIATED 12:28:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED	6 ITERATIONS	1 ANSWERS
SEARCH TIME: 00.00.01		

FULL FILE PROJECTIONS:	ONLINE	**COMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	6 TO	266
PROJECTED ANSWERS:	1 TO	80

L3 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 12:28:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 101 TO ITERATE

100.0% PROCESSED	101 ITERATIONS	22 ANSWERS
SEARCH TIME: 00.00.01		

Kamal Saeed

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L4 22 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
140.28	140.49

FULL ESTIMATED COST

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FILE COVERS 1907 - 9 May 2002 VOL 136 ISS 19
FILE LAST UPDATED: 7 May 2002 (20020507/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l4

L5 5 L4

=> d ibib abs hitstr tot

L5 ANSWER 1 OF 5 CAPIUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:134462 CAPIUS
DOCUMENT NUMBER: 120:134462
TITLE: Heterocyclic phenoxyacetic acid derivative
 antithrombotic and antihypertensive agents
 Hatanaka, Nobuyuki; Takahashi, Kanji; Tokumoto,
 Hideo
INVENTOR(S): Ono Pharmaceutical Co., Ltd., Japan
PATENT ASSIGNEE(S): Eur. Pat. Appl., 112 pp.
SOURCE: CODEN: EPXDXW
 Patent
DOCUMENT TYPE: English
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

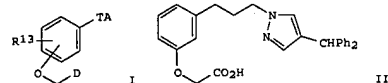
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 558062	A2	19930901	EP 1993-103113	19930226
EP 558062	A3	19940112		
EP 558062	B1	19970507		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT.

SE	CA	AA	CA	1993-2090283	19930224
	JP 2090283	AA 19930829	CA 1993-2090283		19930224
	JP 06055744	A 19404301	JP 1993-59418		19930225
	JP 1362532	B2 20010508			
	JP 200008635	B2 20000328	JP 1999-215729		19930225
	AT 152712	E 19970515	AT 1993-103113		19930226
	ES 2103989	T3 19971001	ES 1993-103113		19930226
	US 5378716	A 19950103	US 1993-24306		19930301
	US 5536736	A 19960716	US 1994-292118		19940819
	US 5703099	A 19971320	US 1996-642598		19960503
	US 5215985	A 19990810	US 1997-925587		19970908
PRIORITY APPLN. INFO.:			JP 1992-78330	A	19920228

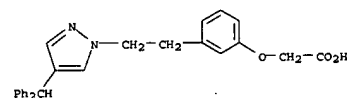
JP 1993-59418	A3	19930225
US 1993-24306	A3	19930301
US 1994-293218	A3	19940819
US 1996-642598	A3	19960503

OTHER SOURCE(S): MARPAT 120:134462
GI

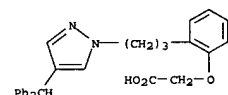


AB The title compounds, I (A = heterocyclyl, carboxylate, (un)substituted CH₂NH₂, etc., D = CO₂R CO₂NR₁R₂, R₁₀ = H, C₁₋₁₂ alkyl; R₁₁, R₁₂ = H, C₁₋₄ alkyl; R₁₃ = H, C₁₋₄ alkyl, C₁₋₄ alkoxy, NO₂; T = direct bond, C₁₋₆ alkylene, C₂₋₆ alkenylene, O(CH₂)₂; s = 2-4), useful in the treatment of thrombosis, arteriosclerosis, ischemic heart disease, gastric ulcer, or hypertension, are prep'd. and 1-*cont.* formulations are presented. Thus,

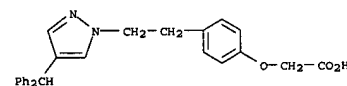
L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



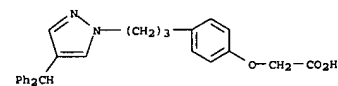
RN 152381-38-9 CAPLUS
CN Acetic acid, [2-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]-
(9CI) (CA INDEX NAME)



RN 152381-40-3 CAPLUS
CN Acetic acid, [4-[2-[4-(diphenylmethyl)-1H-pyrazol-1-yl]ethyl]phenoxy]-
(9CI) (CA INDEX NAME)



RN 152381-41-4 CAPLUS
CN Acetic acid, [4-[3-(4-(diphenylmethyl)-1H-pyrazol-1-yl)propyl]phenoxy]-
(9CI) (CA INDEX NAME)

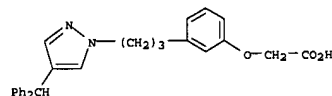


RN 152381-42-5 CAPLUS
CN Acetic acid, [4-[4-[4-(diphenylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy]-
(9CI) (CA INDEX NAME)

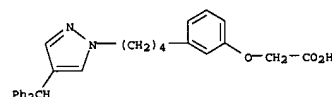
L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)
Me 3-[3-(4-diphenylmethylpyrazol-1-yl)propyl]phenoxyacetate was
hydrolyzed, producing pyrazole deriv. II which demonstrated a 50% human
blood platelet aggregation inhibitory concn. of 0.42 .mu.M.

IT blood platelet aggregation, (antithrombotic and antihypertensive activity of)
 152381-30-1 152381-31-2 152381-35-6
 152381-37-8 152381-38-9 152381-40-3
 152381-41-4 152381-42-5 152381-46-9
 152383-95-0 152383-96-1
 RL: RCT (Reactant)
 (antithrombotic and antihypertensive activity of)

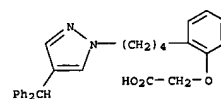
RN 152381-30-1 CAPLUS
 CN Acetic acid, [3-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]-
 (9CI) (CA INDEX NAME)



RN 152381-31-2 CAPLUS
CN Acetic acid, [3-(4-[4-(diphenylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy)-
(9CI) (CA INDEX NAME)

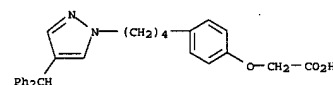


RN 152381-35-6 CAPLUS
CN Acetic acid, [2-(4-[4-(diphenylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy]-
(9CI) (CA INDEX NAME)

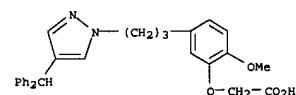


RN 152381-37-8 CAPLUS
CN Acetic acid, {3-[2-[4-(diphenylmethyl)-1H-pyrazol-1-yl]ethyl]phenoxy}-
(9CI) (CA INDEX NAME)

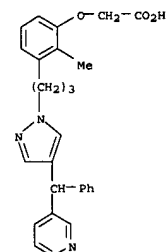
L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 152381-46-9 CAPLUS
CN Acetic acid, [5-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]-2-methoxyphenoxy]- (9CI) (CA INDEX NAME)



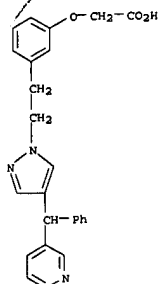
RN 153183-95-0 CAPLUS
CN Acetic acid, [2-methyl-3-[3-[4-(phenyl-3-pyridinylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]- (9CI) (CA INDEX NAME)



RN 153183-96-1 CAPLUS
CN Acetic acid, [3-[2-[4-(phenyl-3-pyridinylmethyl)-1H-pyrazol-1-yl]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

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L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)

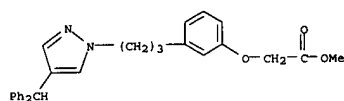


IT 152381-29-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antithrombotic and antihypertensive activities of,
reaction
-OEt)

RN 152381-29-8 CAPLUS

CN Acetic acid, [3-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]-
methyl ester (9CI) (CA INDEX NAME)



IT 152381-30-1P 152381-31-2P 152381-35-6P

152381-37-8P 152381-38-9P 152381-40-3P

152381-41-4P 152381-42-5P 152381-44-7P

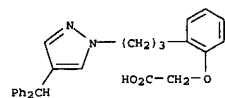
152381-46-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antithrombotic and antihypertensive activity of)

RN 152381-30-1 CAPLUS

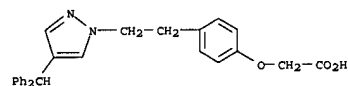
CN Acetic acid, [3-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]-
(9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



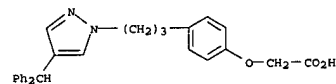
RN 152381-40-3 CAPLUS

CN Acetic acid, [4-[2-[4-(diphenylmethyl)-1H-pyrazol-1-yl]ethyl]phenoxy]-
(9CI) (CA INDEX NAME)



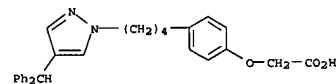
RN 152381-41-4 CAPLUS

CN Acetic acid, [4-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]-
(9CI) (CA INDEX NAME)



RN 152381-42-5 CAPLUS

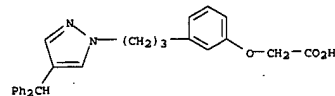
CN Acetic acid, [4-[4-[4-(diphenylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy]-
(9CI) (CA INDEX NAME)



RN 152381-44-7 CAPLUS

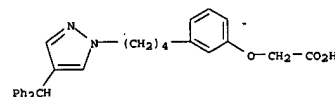
CN Acetic acid, [2-[4-[4-(phenyl-3-pyridinylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy]-
(9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



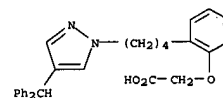
RN 152381-31-2 CAPLUS

CN Acetic acid, [3-[4-[4-(diphenylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy]-
(9CI) (CA INDEX NAME)



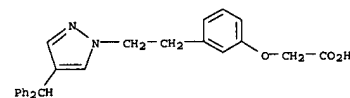
RN 152381-35-6 CAPLUS

CN Acetic acid, [2-[4-[4-(diphenylmethyl)-1H-pyrazol-1-yl]butyl]phenoxy]-
(9CI) (CA INDEX NAME)



RN 152381-37-8 CAPLUS

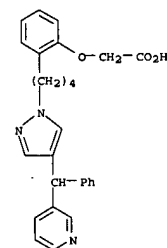
CN Acetic acid, [3-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]ethyl]phenoxy]-
(9CI) (CA INDEX NAME)



RN 152381-38-9 CAPLUS

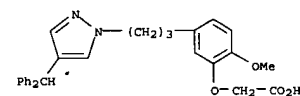
CN Acetic acid, [2-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]phenoxy]-
(9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 152381-46-9 CAPLUS

CN Acetic acid, [5-[3-[4-(diphenylmethyl)-1H-pyrazol-1-yl]propyl]-2-
methoxyphenoxy]- (9CI) (CA INDEX NAME)



1000562

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:134381 CAPLUS

DOCUMENT NUMBER: 120:134381

TITLE: Nonpeptide angiotensin II antagonists derived from 1H-pyrazole-5-carboxylates and 4-aryl-1H-imidazole-5-carboxylates

AUTHOR(S): Ashton, Wallace T.; Hutchins, Steven M.; Greenlee, William J.; Doss, George A.; Chang, Raymond S. L.; Lotti, Victor J.; Faust, Kristie A.; Chen, Tsing Bau; Zingaro, Gloria J.; et al.

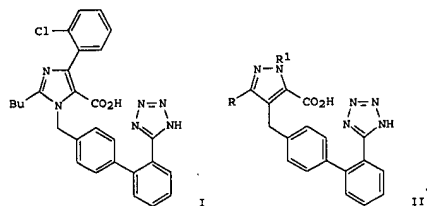
CORPORATE SOURCE: Merck Res. Lab., Rahway, NJ, 07065, USA

SOURCE: J. Med. Chem. (1993), 36(23), 3595-605

DOCUMENT TYPE: Journal

LANGUAGE: English

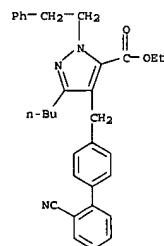
GI



AB Two series of potential angiotensin II antagonists derived from carboxyl-functionalized "diazole" heterocycles have been prepd. and evaluated. Initially, a limited investigation of 4-arylimidazole-5-carboxylates led to 2-n-butyl-4-(2-chlorophenyl)-1-[(2'-(1H-tetrazol-5-yl)biphenyl-4-yl)methyl]-1H-imidazole-5-carboxylic acid (I), which was found to be a highly potent antagonist of the rabbit aorta AT1 receptor (IC50 0.55 nM). In conscious, normotensive rats, I at 0.1 mg/kg i.v. inhibited the pressor response to AII by 88%, with a duration of >6 h. More extensively studied was an isosteric series of 3-alkyl-4-[(2'-(1H-tetrazol-5-yl)biphenyl-4-yl)methyl]-1H-pyrazole-5-carboxylates bearing aryl, alkyl, or aralkyl substituents at N1. These compds. were available in highly regioselective fashion via condensation of a substituted hydrazine hydrochloride with a 2-(methoxyimino)-4-oxoalkanoate intermediate. In vitro, the most potent pyrazolecarboxylic acids were II (R = Bu; R1 = 2,6-dichlorophenyl, 2-(trifluoromethyl)phenyl, benzyl, and phenethyl), all with IC50 values of 0.18-0.24 nM. Although less potent

in the receptor assay, 3-n-propylpyrazolecarboxylic acids were at least as effective as their Bu counterpart in vivo. Several of the pyrazolecarboxylic acid deriva. demonstrated potent, long-lasting oral activity in rats. At 1 mg/kg po, the II (R = Bu, R1 = benzyl; R = Pr, R1

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)

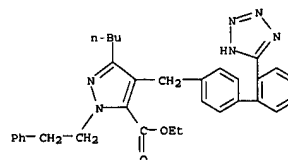
= 2,6-dichlorophenyl, 2,2,2-trifluoroethyl, and benzyl) analogs all gave >75% inhibition of the AII pressor response in the rat model, with duration of action >23 h.

IT 152713-37-6P 152713-50-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and angiotensin II antagonist activity of)

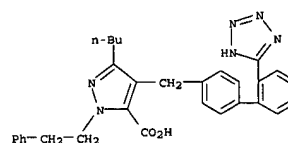
RN 152713-37-6 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-1-(2-phenylethyl)-4-[(2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 152713-50-3 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-1-(2-phenylethyl)-4-[(2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]- (9CI) (CA INDEX NAME)



IT 152713-71-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and cyclization of, with azide, triazole deriv. from)

RN 152713-71-8 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-4-[(2'-cyano[1,1'-biphenyl]-4-yl)methyl]-1-(2-phenylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

the receptor assay, 3-n-propylpyrazolecarboxylic acids were at least as effective as their Bu counterpart in vivo. Several of the pyrazolecarboxylic acid deriva. demonstrated potent, long-lasting oral activity in rats. At 1 mg/kg po, the II (R = Bu, R1 = benzyl; R = Pr, R1

L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:603377 CAPLUS

DOCUMENT NUMBER: 119:203377

TITLE: reaction of N-substituted acetohydrazides with 2-substituted cinnamitriles. Competitive cyclizations to pyrazolo[3,4-b]pyridinones and [1,2,4]triazolo[1,5-a]pyridinones

AUTHOR(S): Hadi, Ali; Martin, Nazario; Seoane, Carlos; Soto, Jose

CORPORATE SOURCE: Fac. Quim., Univ. Complutense, Madrid, 28040, Spain

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1993), (9), 1045-50

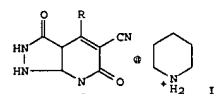
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 119:203377

GI



AB A novel prepn. of pyrazolo[3,4-b]pyridinones I (R = aryl) from 2'-acyl-2-cyanoacetohydrazide and arylidenecyanoacetates is described.

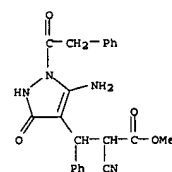
In the reaction, an alternative cyclization, leading to [1,2,4]triazolo[1,5-a]pyridinones takes place. Compds. I were isolated from the reaction mixt. as the corresponding.

IT 150568-54-0P 150568-55-1P 150568-57-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 150568-54-0 CAPLUS

CN 1H-Pyrazole-4-propanoic acid, 5-amino-.alpha.-cyano-2,3-dihydro-3-oxo-.beta.-phenyl-1-(phenylacetyl)-, methyl ester (9CI) (CA INDEX NAME)



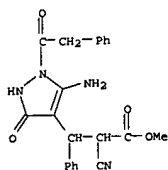
RN 150568-55-1 CAPLUS

CN 1H-Pyrazole-4-propanoic acid, 5-amino-.alpha.-cyano-2,3-dihydro-3-oxo-.beta.-phenyl-1-(phenylacetyl)-, methyl ester, compd. with piperidine

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L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)
(1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 150568-54-0
CMP C22 H20 N4 O4

CM 2

CRN 110-89-4
CMP C5 H11 NRN 150568-57-3 CAPLUS
CN 1H-Pyrazole-4-propanoic acid, 5-amino-2,3-dihydro-3-oxo-1-phenyl-1-(phenylacetyl)-, ethyl ester, compd. with piperidine
(1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 150568-56-2
CMP C23 H22 N4 O4

L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:539046 CAPLUS
DOCUMENT NUMBER: 109:139046
TITLE: Silver halide photographic material containing yellow coupler
INVENTOR(S): Tsuruta, Mayumi; Mizukura, Noboru; Nakagawa, Satoshi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAP
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63092951	A2	19880423	JP 1986-238222	19861007

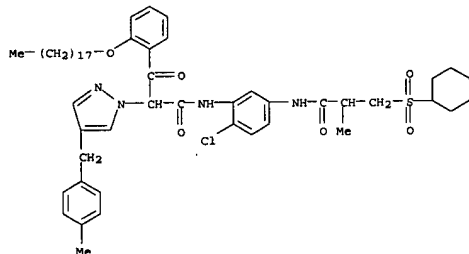
GI For diagram(s), see printed CA Issue.

AB In the title photog. material, .gtoreq.1 of photog. Ag halide emulsion layers contains a yellow coupler I [R1 = alkyl, cycloalkyl, aryl; R2 = group which can be substituted to the benzene ring; R3 = H, alkyl, aryl, heterocyclyl; X = alkylene, cycloalkylene, arylene, alkylene arylene, arylene alkylene, or -A-V-B (A, B = alkylene, arylene, alkylenearylene, or arylenealkylene; V = divalent connecting group); Y = alkyl, cycloalkyl, aryl, heterocyclyl; Z = nonmetal atoms to form a 5- or 6-membered ring with -N(CO)n-; m = 0, 1; n = 0-2]. The photog. material shows improved color-forming d., reduced fog, and improved storage stability.

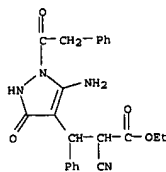
IT 116624-91-0
RL: TEM (Technical or engineered material use); USES (Uses)
(photog. yellow coupler)

RN 116624-91-0 CAPLUS

CN 1H-Pyrazole-1-acetamide,
N-[2-chloro-5-[[3-(cyclohexylsulfonyl)-2-methyl-1-oxopropyl]amino]phenyl]-4-[[4-methylphenyl)methyl]-.alpha.-(2-octadecyloxy)benzoyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)

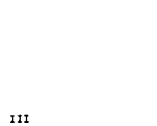
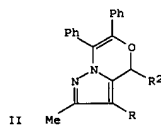
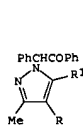


CM 2

CRN 110-89-4
CMP C5 H11 N

L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1984:423412 CAPLUS
DOCUMENT NUMBER: 101:23412
TITLE: Reactions of azines. 8. Synthesis and thermal rearrangement of 1-oxo-3,4-diaza-2,4,6-heptatrienes and 1-oxo-3,4-diaza-2,4,6,7-octatetraenes (allenyl azines)
AUTHOR(S): Schweizer, Edward E.; Lee, Kee Jung
CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19711, USA
SOURCE: J. Org. Chem. (1984), 49(11), 1959-64
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:23412
GI

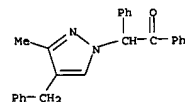


AB Cycloaddn. reactions of 1-oxo-3,4-diaza-2,4,6-heptatrienes, obtained from PhCOCPh:NN:CMcCR:PPH3 (I; R = Me, Et, Pr, H2C:CHCH2, PhCH2), with aldehydes gave substituted pyrazoles II (R = Me, R1 = Ph, p-O2NC6H4; R = Et, Pr, R1 = p-O2NC6H4; R = H2C:CHCH2 R1 = Ph; R = PhCH2, R1 = H) in 66-89% yield. I (R = PhCO) failed in the olefination reaction, giving only the corresponding acetylene. A similar allenylation reaction of I (R = Me, H2C:CHCH2, PhCH2) with R2HC:CO (R2 = H, Ph, PhCH2) gave pyrazolo[5,1-c][1,4]oxazines III in 65-81% yield via the intermediate 1-oxo-3,4-diaza-2,4,6,7-octatetraenes. I (R = PhCO) only reacted with H2C:CO to give III in 21% yield.

IT 89849-25-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 89849-25-2 CAPLUS

CN Ethanone, 2-[3-methyl-4-(phenylmethyl)-1H-pyrazol-1-yl]-1,2-diphenyl- (9CI) (CA INDEX NAME)



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=> file reg

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

23.93

164.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

ENTRY

TOTAL

SESSION

CA SUBSCRIBER PRICE

-3.10

-3.10

FILE 'REGISTRY' ENTERED AT 12:31:45 ON 09 MAY 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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STRUCTURE FILE UPDATES: 7 MAY 2002 HIGHEST RN 412267-09-5

DICTIONARY FILE UPDATES: 7 MAY 2002 HIGHEST RN 412267-09-5

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\Program Files\Stnexp\Queries\0989932211.str

L6 STRUCTURE UPLOADED

=> que L6

L7 QUE L6

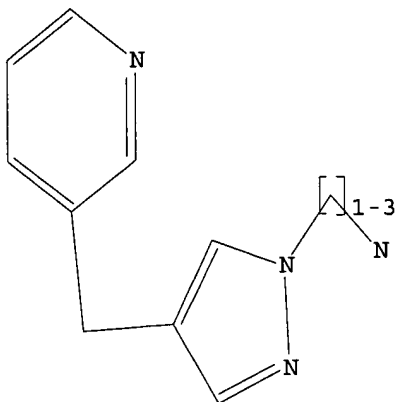
=> d

L7 HAS NO ANSWERS

L6 STR

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Structure attributes must be viewed using STN Express query preparation.
L7 QUE ABB=ON PLU=ON L6

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=> s l6
SAMPLE SEARCH INITIATED 12:32:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE
```

```
100.0% PROCESSED      0 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   0 TO      0
PROJECTED ANSWERS:      0 TO      0
```

L8 0 SEA SSS SAM L6

```
=> s l1 full
FULL SEARCH INITIATED 12:33:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 101 TO ITERATE
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100.0% PROCESSED      101 ITERATIONS      22 ANSWERS
SEARCH TIME: 00.00.01
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L9 22 SEA SSS FUL L1

```
=> s l7 full
FULL SEARCH INITIATED 12:33:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8 TO ITERATE
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100.0% PROCESSED      8 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.02
```

L10 0 SEA SSS FUL L6

```
=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
```

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COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

280.94

445.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY

TOTAL
SESSION

CA SUBSCRIBER PRICE

0.00

-3.10

STN INTERNATIONAL LOGOFF AT 12:33:49 ON 09 MAY 2002

Kamal Saeed